

## ABSTRACT

A method for characterizing the three-dimensional surface  
5 structure of molecules, particularly proteins and protein  
complexes, employing mass spectrometric analysis, an electrospray  
ionization (ES) source, a novel data interpretation process that  
utilizes comparisons of particular binding constants ( $K_b$ ) and  
heats of formation ( $\Delta H_f$ ), and computational feedback modeling.

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